Theoretical and Experimental Chemistry 1987 vol.23 N2, pages 150-158

The nature of "anomalous" chemical shifts in certain heterocycles based on nonempirical calculations and localization

Aminova R., Samitov Y.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

The method of gradient invariant atomic orbitals with expansion by Gaussian functions has been used to compute the diagrams for magnetic isoshielding lines in the vicinity of unshared electron pairs of an oxygen atom and the C-O bond. From localized molecule orbitals the chemical shift in 1,3-dioxane has been analyzed. A nonempirical calculation has been made of the electronic structure of a number of six-membered heterocycles and a qualitative correlation has been established between the relative charges and the chemical shifts. © 1987 Plenum Publishing Corporation.

http://dx.doi.org/10.1007/BF00534574